A Geospatial Model for Remedial Design Optimization and Performance Evaluation

V.M. Madrid, Z. Demir, S. Gregory, J. Valett, R.U. Halden

This article was submitted to The Battelle, Remediation of Chlorinated and Recalcitrant Compounds: The Third International Conference, Monterey, CA, May 20 – 23, 2002

U.S. Department of Energy



February 1, 2002

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

This work was performed under the auspices of the United States Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

This report has been reproduced directly from the best available copy.

Available electronically at http://www.doc.gov/bridge

Available for a processing fee to U.S. Department of Energy
And its contractors in paper from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062

Telephone: (865) 576-8401 Facsimile: (865) 576-5728 E-mail: reports@adonis.osti.gov

Available for the sale to the public from U.S. Department of Commerce National Technical Information Service 5285 Port Royal Road Springfield, VA 22161 Telephone: (800) 553-6847 Facsimile: (703) 605-6900

E-mail: <u>orders@ntis.fedworld.gov</u>
Online ordering: <u>http://www.ntis.gov/ordering.htm</u>

OR

Lawrence Livermore National Laboratory
Technical Information Department's Digital Library
http://www.llnl.gov/tid/Library.html

A GEOSPATIAL MODEL FOR REMEDIAL DESIGN OPTIMIZATION AND PERFORMANCE EVALUATION

Victor M. Madrid (madrid2@llnl.gov), Zafer Demir, and Steven Gregory (Lawrence Livermore National Laboratory, Livermore, CA, USA),
John Valett (Weiss Associates, Emeryville, CA, USA)
Rolf U. Halden (Johns Hopkins University, Bloomberg School of Public Health,
Baltimore, MD, USA)

ABSTRACT: Soil and ground water remediation projects require collection and interpretation of large amounts of spatial data. Two-dimensional (2D) mapping techniques are often inadequate for characterizing complex subsurface conditions at contaminated sites. To interpret data from these sites, we developed a methodology that allows integration of multiple, three-dimensional (3D) data sets for spatial analysis. This methodology was applied to the Department of Energy (DOE) Building 834 Operable Unit at Lawrence Livermore National Laboratory Site 300, in central California. This site is contaminated with a non-aqueous phase liquid (NAPL) mixture consisting of trichloroethene (TCE) and tetrakis (2-ethylbutoxy) silane (TKEBS). In the 1960s and 1970s, releases of this heat-exchange fluid to the environment resulted in TCE concentrations up to 970 mg/kg in soil and dissolved-phase concentrations approaching the solubility limit in a shallow, perched water-bearing zone. A geospatial model was developed using site hydrogeological data, and monitoring data for volatile organic compounds (VOCs) and biogeochemical parameters. The model was used to characterize the distribution of contamination in different geologic media, and to track changes in subsurface contaminant mass related to treatment facility operation and natural attenuation processes. Natural attenuation occurs mainly as microbial reductive dechlorination of TCE which is dependent on the presence of TKEBS, whose fermentation provides the hydrogen required for microbial reductive dechlorination of VOCs. Output of the geospatial model shows that soil vapor extraction (SVE) is incompatible with anaerobic VOC transformation, presumably due to temporary microbial inhibition caused by oxygen influx into the subsurface. Geospatial analysis of monitoring data collected over a three-year period allowed for generation of representative monthly VOC plume maps and dissolved-phase mass estimates. The latter information proved to be invaluable in optimizing and evaluating the remedial design and performance.

INTRODUCTION

Environmental cleanup projects involve the collection and interpretation of large amounts of interdisciplinary spatial data. These data are used to 1) characterize the nature and extent of subsurface contamination, 2) develop cost-effective, media-specific remedial strategies, 3) monitor the cleanup progress, and 4) demonstrate to regulatory agencies that further risk to human health and natural resources is properly managed. The ability to integrate different types of data into a geospatial model of the subsurface is

crucial to the success of any soil and ground water cleanup effort (Bruckner and Schneider, 2001).

In this paper, we present a geospatial model that was developed using EarthVision software (Dynamic Graphics, Inc, 1999) to visualize and integrate multiple independent data sets from a site that contains trichloroethylene (TCE) as a Dense Non-Aqueous Phase Liquid (DNAPL). In addition to the primary volatile organic compound (VOC) TCE, its daughter product *cis*-1,2 dichloroethene (*cis*-1,2-DCE) is also present as a result of microbial reductive dechlorination activity. Previous studies have shown that the microbial reductive dechlorination of TCE to *cis*-1,2-DCE can be linked to the presence of TKEBS, that was released to the environment along with TCE as a mixture (Halden *et al.*, 1999). Fermentation of TKEBS yields the hydrogen required for microbial reductive dechlorination of VOCs This anaerobic process is inhibited by the influx of oxygen to the subsurface during soil vapor extraction (SVE). A geospatial model was developed to optimize the remedial design and evaluate the performance of the remediation system (Gregory *et al.*, 2001).

METHODS

Our approach to data analysis is based on the integration of different data sets into a geospatial model using EarthVision to characterize and evaluate subsurface conditions. The first step is to review the quality of each data set to ensure that it is representative of subsurface conditions. The second step is an iterative process whereby the conceptual model is repeatedly tested and improved as different data sets are integrated. The third step is a media-specific spatial analysis that includes saturated-unsaturated, low, medium, and high hydraulic conductivity zones.

We used two types of models (structure and property models) for spatial analysis. Structure modeling was used to analyze geologic, hydrologic, and ground water chemical data. Property modeling was used to interpolate, visualize, and analyze the 3D distribution of properties, such as soil contaminant concentration and hydraulic conductivity, within each geologic unit. Five separate geospatial models were developed to analyze data from the Building 834 site. The five models include, three structure models (geologic, hydrologic, and dissolved contaminant distribution) and two 3D property models (lithology and soil contaminant distribution). These models were incorporated into a comprehensive contaminant-hydrogeologic model to optimize remedial design, and to evaluate treatment system performance and intrinsic bioremediation.

ANALYSIS

Property Modeling for Remedial Design Optimization. A lithologic property model was developed to characterize the 3D distribution of high-, medium-, and low-K materials. These lithologic groupings are based on visual inspection of core samples collected from 30 boreholes drilled to a maximum depth of 90 feet. Each lithology was assigned a numerical value for spatial interpolation using a minimum-tension gridding algorithm.

A second property model was developed based on the 3D distribution of soil contaminant concentrations. Two separate data sets were incorporated into the soil contaminant property model: 1) soil chemical concentrations (TCE in mg/kg) from over

300 soil samples, and 2) passive soil vapor data using GORE sorbers. Only non-detect GORE sorber data were used to accurately define the outer limits of soil contamination.

These two 3D property models were integrated into a soil contaminant distribution model to characterize the 3D distribution of contaminants and estimate soil contaminant mass in the three lithologic zones. Results from the soil contaminant model are presented in Figure 1A and 1B. Figure 1A shows the distribution of soil contaminants in the high-K zones and Figure 1B shows the distribution in the low-K zones. The soil property data are presented on these images as color-coded well tubes and the distribution is shown as color-filled shells of equal soil concentration.

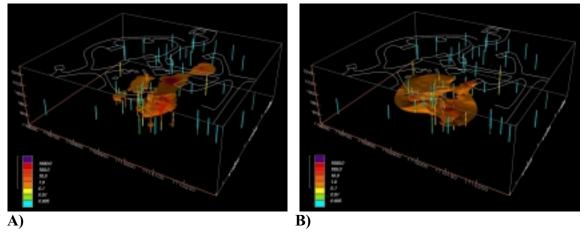


FIGURE 1. Combined soil contamination and lithology models showing A) high-K and B) low-K zones.

As a result of this analysis we selected media-specific remedial technologies that are based on contaminant mass estimated for each soil type (high-, medium-, and low-K) using property volumetric analysis (Figure 2). The region displayed in Figure 1A represents the primary target for SVE. New targets for SVE were identified and additional SVE wells are now planned. The presence of high soil contaminant concentrations in clay-rich, low-K zones (Figure 1B), limits the effectiveness of the current treatment system because these zones function as long-term sources. Innovative remediation techniques, such as enhanced bioremediation, may be required to cleanup these zones.

Contaminant-Hydrogeologic Modeling for Remedial Performance Evaluation. A contaminant-hydrogeologic model was developed to evaluate the performance of the ground water and SVE system. From January 1998 to December 2000, dissolved contaminant mass changes related to ground water storage and treatment system operations were tracked.

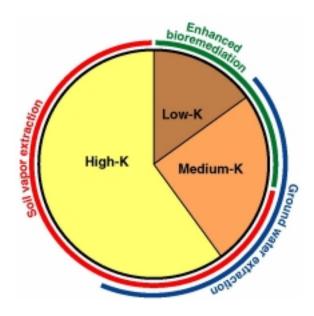


FIGURE 2. Relative distribution of contaminant mass in different geologic media and selected media-specific remedial strategy.

The geologic model is based on integrating surface and subsurface geologic data, including lithologic descriptions from borehole samples and continuous cores, geophysical logs, optical televiewer data, and outcrops. The geologic model contains three layers. In descending order: 1) a 20- to 30-foot thick sand and gravel layer, 2) a 10to 20-foot thick clay layer or perching horizon, and 3) a bedrock layer. The hydrologic model is based on rainfall and representative ground water elevation data collected from wells screened in the water-bearing sand and gravel layer. Water level data from each well were examined to develop representative hydrographs that reflect formation conditions. The purpose of the hydrologic model is to characterize spatial and temporal changes in extent of saturation and ground water storage for volumetric analysis. The contaminant distribution model is based on representative ground water chemical concentrations. Chemical data from each well were examined to develop representative time-series plots of various chemical and biogeochemical parameters. The purpose of the contaminant distribution model is to track spatial and temporal changes in dissolved phase VOC mass. A volumetric analysis was performed using the saturated thickness from the hydrologic model and contaminant distribution from the contaminant model. Figures 3A and 3B depict the distribution of dissolved Total VOCs and cis-1,2-DCE during unstressed and stressed conditions.

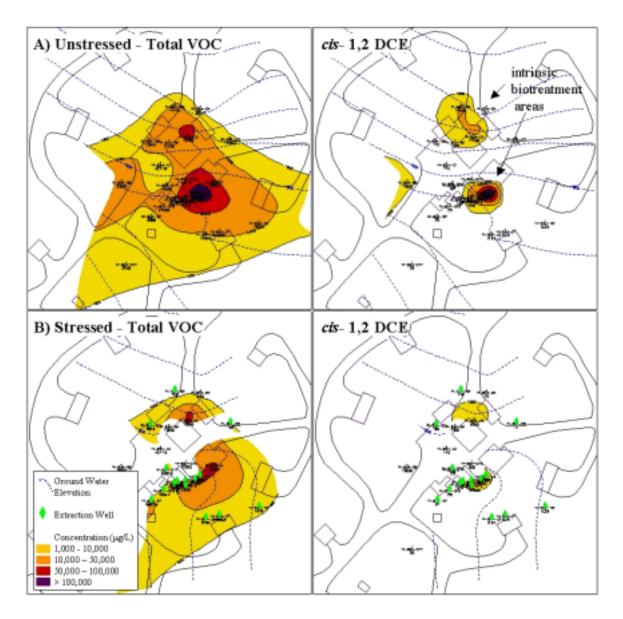


FIGURE 3. Maps of ground water elevation, Total VOC, and *cis*-1,2-DCE for A) unstressed and B) stressed conditions.

RESULTS

Remediation System Performance Evaluation. The results of volumetric analysis and dissolved-phase contaminant mass tracking are presented as two time-series plots in Figures 4A and 4B. Figure 4A shows that dissolved contaminants reached a maximum level of 82 kg in March 1998 following the El Niño rainfall events of January and February. Following these events, the treatment facility was operated from May 1998 to June 1999, on an 8-hour/day and 5days/week basis. Volumetric analysis indicates that dissolved contaminant mass decreased by 59 kg or 72% between May 1998 and May 1999. Treatment facility mass removal data, shown in Figure 4B, indicate that 9 kg of VOCs were removed by ground water extraction and 23 kg were removed by soil vapor extraction, yielding a total of 32 kg removed. The difference between the mass removed

by the treatment facility and the estimated reduction in dissolved-phase mass indicates that a significant amount of the VOC mass remains in the vadose zone as water levels decline.

From August 1999 to January 2000, the treatment facility was operated on a continuous 24-hour basis. Volumetric analysis indicates that subsurface dissolved-phase contaminant mass decreased by 6.5 kg from 15 kg in August 1999 to 8.5 kg in January 2000. Treatment facility mass removal data indicate that 2.5 kg of VOCs were removed from extracted ground water and 36 kg were extracted in the vapor phase, yielding a total of 38.5 kg removed. These data indicate that nearly all of the mass removal was accomplished by the SVE system. Of the 36 kg removed in the vapor phase, 4 kg was removed via volatilization of contaminants dissolved in ground water and the remaining 34.5 kg was removed from the vadose zone.

Evaluation of Intrinsic Bioremediation. Treatment facility operations were temporarily discontinued to evaluate the extent of natural VOC attenuation processes, mainly intrinsic bioremediation. Two intrinsic bioremediation evaluation tests were conducted under different seasonal conditions; the first under dry, summer conditions, and the second under wet, winter conditions. During both tests, rapid changes in Eh, dissolved oxygen, and *cis*-1,2 DCE concentrations were observed in specific wells. These wells are located in areas (intrinsic biotreatment areas) that contain TCE mixed with the silicon-based oil, TKEBS. TCE concentrations in the intrinsic biotreatment areas decreased by one to two orders of magnitude, while *cis*-1,2-DCE concentrations increased by the same magnitude. Evidence of anaerobic dechlorination beyond *cis*-1,2-DCE (*e.g.*, vinyl chloride), however, was not observed at 100 μg/L detection limit.

During the summer test, treatment facility operations were discontinued for about two months, from mid-June to mid-August, 1999. As shown in Figure 4B, a significant decrease in dissolved VOC mass (6.5 kg) was observed that may be partly or entirely due to intrinsic bioremediation. The winter test was conducted from February to May 2000 during rainfall events. As shown in Figure 4B, dissolved-phase VOC mass increased from 8 kg to 24 kg during the first three months of the test and then remained relatively constant until May. The increase in dissolved VOC mass is mainly due to increase in ground water storage and source dissolution.

CONCLUSIONS

We developed a geospatial model to visualize subsurface data, optimize remedial design, and evaluate remedial performance at a complex site where ground water and soil vapor extraction and treatment technologies are being used to clean up a DNAPL-source area. Spatial analysis resulted in new targets for SVE and identified significant contaminant mass in fine-grained, clay-rich sediments, which will require enhanced remediation techniques for cleanup. Geospatial modeling was also used to evaluate remedial performance by tracking changes in dissolved VOC mass in ground water related to treatment facility operations, source dissolution, and natural attenuation processes.

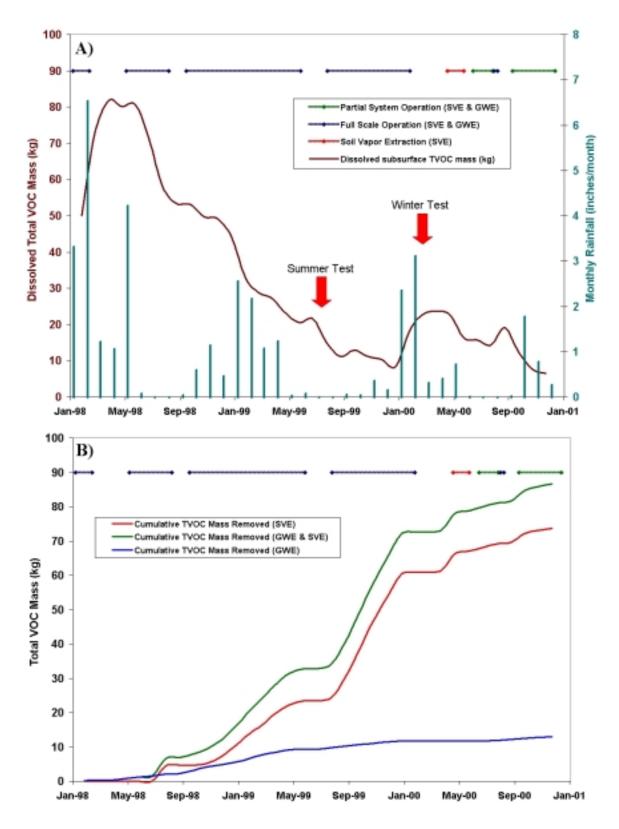


FIGURE 4. Time-series plots of A) dissolved-phase volatile organic compound mass remaining in ground water and B) treatment facility cumulative mass removal data.

Intrinsic bioremediation was evaluated under both summer and winter conditions. Although intrinsic bioremediation occurs within limited biotreatment areas, significant overall mass reduction was observed during the summer test. An observed net increase in dissolved-phase mass during the winter rainfall and recharge events, however, most likely is due to source dissolution rates that far exceed the rate of VOC loss caused by intrinsic bioremediation. An expansion of the biotransformation zone via nutrient addition (enhanced bioremediation) may be a viable remedial alternative for final cleanup at this site, once the current treatment technologies are no longer cost effective.

ACKNOWLEGMENTS

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

REFERENCES

Bruckner, A.E., and W.H. Schneider. 2001. "Using Geospatial Models and 3-D Visualization to Advance Decision-making and Communication of Remedial Solutions to Environmental Programs", *Proceedings of the A&WMA 94th Annual Conference, Orlando, Florida*.

Dynamic Graphics, Inc., Alameda California. 1999 "EarthVision User's Guide, Version 5.1".

Gregory, S.D., V.M.. Madrid, L. Ferry, R.U. Halden, and Z. Demir. 2001. *Interim Remedial Design for the Building 834 Operable Unit Treatment Facility at Lawrence Livermore National Laboratory Site 300*. Lawrence Livermore National Laboratory, Livermore, Calif. UCRL-AR-144919.

Halden, R.U., V.M.. Madrid, P.F. Daley, M. Lima, S.D. Gregory, and J.P. Ziagos. 1999. "Silicone Lubricants Facilitate Bioattenuation of TCE at LLNL's Superfund Site 300", Proceedings of the Fifth International Symposium for In Situ and On-Site Bioremediation, San Diego, California.